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Screen the best ionic liquids for keratin dissolution by using COSMO-RS

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Wool keratin is a kind of degradable natural biopolymer and extensively used in the textile and biomedical fields. But keratin is hard to reuse because it is difficult to dissolve in conventional solvents. An increasing interest has been manifested in the use of ionic liquids (ILs) as solvents for dissolution of wool keratin due to their tuneable and excellent properties. However, it is nevertheless a challenge to identify the best ILs for keratin dissolution. Experimental measurement of all these systems is not practically feasible; hence a rapid and a priori screening method to predict the keratin solubility capacity for ILs is needed. Based on our previous work, we designed three models for describing wool keratin, and 462 ILs formed from 21 cations and 22anions were selected for evaluation of their ability to dissolve wool keratin by COSMO-RS. From the prediction results of logarithmic activity coefficients (lnγ) of the three keratin models, it can be concluded that keratin dissolution capacity is mostly determined by the anion while the cation only has a moderate effect on the dissolution process. Ac^-, Dec^-, $HCOO^-$, Cl^-, BEN^-, DMP^-, DEP^-, DBP^-, TOS^- and $Br^-$with various cations studied in this work exhibited particularly good properties for keratin dissolution. The excess enthalpy calculations indicated that the main forces in the keratin dissolution in ILs are H-bonds, while the contribution of misfit forces and van der Waals forces are secondary.

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